An introduction to quantum Monte Carlo cluster algorithms

Matthias Troyer (ETH Zürich)

Classical cluster algorithms
Quantum Monte Carlo
- Path integrals
- Stochastic Series Expansion
Quantum Cluster algorithms
- Loop algorithm
- Worm algorithm
Wang-Landau sampling
- allows tunneling through free energy barriers
- efficient for 1st order transitions and spin glasses

What can cluster algorithms do?

♦ Local updates (before 1994)
  ♦ 200 spins
  ♦ T=0.1

♦ Cluster algorithms (after 1995)
  ♦ 2D quantum phase transition: 20’000 spins at T=0.005
  ♦ 2D square lattice: 1’000’000 spins at T=0.2
  ♦ 3D antiferromagnet 16’000’000 spins at T=1 (Sandvik)

♦ Cluster algorithms allow to reach asymptotic scaling regime
  ♦ Accurate estimates of critical exponents
  ♦ Check of scaling predictions
Our applications

- Quasi-1D spin systems
  - Ladders, chains, spin-orbital models
- 2D+3D antiferromagnets
  - Quantum phase transition sin Heisenberg models
  - Magnetic field effects (quantum Hall bilayers)
  - Impurity doping
- 2D bosons
  - Solids, supersolids, smectics, nematics
  - Dirty hardcore bosons
  - Trapped bosons (BEC in optical lattice)
- Realistic modeling
  - 2D vanadates
  - Coupled cuprate and vanadate ladders
- Current and future
  - Search for spin liquids in SU(N) antiferromagnets
  - Dissipation-driven phase transitions
  - Quantum spin glasses
  - Trapped atomic condensates in optical lattices

S=1 square lattice: nickelates

- Quantum field theory:
  \[
  \frac{\xi}{a} = \frac{e^{\frac{T}{k_B} / a}}{8 \pi \xi} \exp \left( \frac{2 \pi \rho_s}{k_B T} \right) \left[ 1 - \frac{1}{2} \frac{k_B T}{2 \pi \rho_s} + O \left( \frac{k_B T}{4 \pi \rho_s} \right) \right] + \ldots
  \]

- Semi-classical PQSCHA
  - Cuccoli et al., PRL 1996, PRB 1997
  - Quantum effects renormalize the temperature
  \[
  \xi = \xi_{\text{classical}} (T)
  \]

- Quantum effects weak for spin $S>1/2$
  - Semi-classical description applicable
S=1/2 square lattice: cuprates

- Quantum field theory
  \[ \xi = \frac{c}{a} \exp \left( \frac{2\pi}{k_B T} \left( 1 - \frac{1}{2} \frac{k_B T}{\xi_{\text{classical}}} \right) \right) + \ldots \]

- Semi-classical PQSCHA
  - Cuccoli et al., PRL 1996, PRB 1997
  - quantum effects renormalize the temperature
  \[ \xi = \xi_{\text{classical}}(f_S(T)) \]
  - Quantum effects important for spin S=1/2

Spin ladder materials

- are coupled dimers
- Numerical simulations show that spin gap survives coupling, no ordering
- Quantitative fits of models to experimental measurements are possible
An Introduction to Quantum Monte Carlo Cluster Algorithms

Phase diagram of 2D hard core bosons

- Unusual reentrant behavior
  - Normal fluid
  - Solid
  - Normal fluid
  - Superfluid

- Three melting transitions
  - Second order into normal fluid
  - First order into normal fluid
  - First order into superfluid

Classical Monte Carlo simulations

- We want to calculate a thermal average
  \[ \langle A \rangle = \sum_c A_c e^{-\beta E_c} / Z \]
  with \( Z = \sum e^{-\beta E_c} \)

- Exponentially large number of configurations
  \( \Rightarrow \) draw a representative statistical sample by importance sampling

- Pick \( M \) configurations \( c_i \) with probability

- Calculate statistical average

- Within a statistical error

- Problem: we cannot calculate

\[ p_{c_i} = e^{-\beta E_{c_i}} / Z \] since we do not know \( Z \)
Markov chains and Metropolis algorithm

- Metropolis algorithm builds a Markov chain
  \[ c_1 \rightarrow c_2 \rightarrow ... \rightarrow c_i \rightarrow c_{i+1} \rightarrow ... \]

- Transition probabilities \( W_{x,y} \) for transition \( x \rightarrow y \) need to fulfill
  - Ergodicity: any configuration reachable from any other
    \[ \forall x, y \exists n : (W^n)_{x,y} \neq 0 \]
  - Detailed balance:
    \[ \frac{W_{x,y}}{W_{y,x}} = \frac{p_y}{p_x} \]

- Simplest algorithm due to Metropolis (1953):
  \[ W_{x,y} = \min[1, \frac{p_y}{p_x}] \]

- Needs only relative probabilities (energy differences)
  \[ \frac{p_y}{p_x} = e^{-\beta(E_y-E_x)} \]

Critical slowing down of local updates

- Autocorrelations in Markov chain change error estimate:
  \[ \Delta A = \sqrt{(\langle A - \langle A \rangle \rangle)^2} = \sqrt{\frac{\text{Var}A}{M} \left(1 + 2\tau_a \right)} \]

- Autocorrelation time \( \tau_a \) diverges at criticality (critical slowing down)
  \[ \tau \propto \min[\xi, L] \]

- Local spin flips: \( z=2 \Rightarrow \) effort increased by \( L^2 \)

- Advantage of Monte Carlo simulations
  - Can change the dynamics!
  - Dynamical exponent is non-universal
  - Need improved dynamics that change the system on length scale \( \xi \)
Cluster Algorithms: the simple explanation

♦ For each spin we ask: “do we want to change its alignment with its neighbors?”
  ♦ Antiparallel spins gain energy ⇒ can change it
  ♦ Parallel spins lose energy
    ♦Accepted only with probability \(\exp(-2\beta J)\) (introduce a domain wall)
    ♦ Otherwise we also have to flip its neighbor ⇒ we add the neighbor to the cluster with probability \(1 - \exp(-2\beta J)\)

Can be extended to cluster representation of the partition function

Cluster algorithms: the formal explanation

♦ We extend the phase space
  ♦ From configurations \(C\) to configurations + graphs \((C,G)\)

\[
Z = \sum_C W(C) = \sum_C \sum_G W(C,G) \text{ with } W(C) = \sum_G W(C,G)
\]

♦ Choose graph weights independent of configuration

\[
W(C,G) = \Delta(C,G)V(G) \text{ where } \Delta(C,G) = \begin{cases} 1 & \text{graph } G \text{ allowed for } C \\ 0 & \text{otherwise} \end{cases}
\]

♦ Perform updates
  1. Pick a graph \(G\) \(P[G] = \frac{V(G)}{W(C)}\)
  2. Discard configuration
  3. Pick any allowed new configuration
  4. Discard graph

Detailed balance

\[
\frac{P(C,G) \rightarrow (C',G)}{P(C',G) \rightarrow (C,G)} = \frac{1/N_C}{1/N_C} = \frac{\Delta(C,G)V(G)}{\Delta(C',G)V(G)} = \frac{P((C',G))}{P((C,G))}
\]
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Cluster algorithms: Ising model

- We need to find $\Delta(C, G)$ and $V(G)$ to fulfill:

$$W(C) = \sum_{G} W(C, G) = \sum_{G} \Delta(C, G) V(G)$$

<table>
<thead>
<tr>
<th>$\Delta(C, G)$</th>
<th>$W(C)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\uparrow\uparrow, \downarrow\downarrow$</td>
<td>1</td>
</tr>
<tr>
<td>$\uparrow\downarrow, \downarrow\uparrow$</td>
<td>0</td>
</tr>
</tbody>
</table>

- $W(G)$

$$e^{+\beta J} - e^{-\beta J}$$

- $e^{-\beta J}$

- This means for:
  - Parallel spins: pick connected graph $\uparrow\uparrow$ with
  - Antiparallel spins: always pick open graph $\downarrow\downarrow$

- And for: $G \rightarrow (C_{\text{rel}}, G) \rightarrow C_{\text{rel}}$
  - Configuration must be allowed $\Rightarrow$ connected spins must be parallel
  - $\Rightarrow$ connected spins flipped as one cluster

Quantum Monte Carlo

- Not as easy as classical Monte Carlo

$$Z = \sum_{\epsilon} e^{-\beta H_\epsilon}$$

- Calculating the energy eigenvalue $E_\epsilon$ is equivalent to solving the problem

- Need to find a mapping of the quantum partition function to a classical problem

$$Z = \text{Tr} e^{-\beta H} = \sum_{\epsilon} p_\epsilon$$

- Two approaches
  - Path integrals (time-dependent perturbation theory in imaginary time)
  - Series Expansion

- Sign problem if some $p_\epsilon < 0$
Path Integral Representation

- Interaction representation
  \[ H = H_0 + V, \quad H_0 = \sum_{<i,j>} J_{ij} S_i^z S_j^z, \quad V = \sum_{<i,j>} J_{ij}^\text{ex} (S_i^x S_j^x + S_i^y S_j^y) \]
  \[ Z = \text{Tr}(e^{-\beta H}) = \text{Tr}(e^{-\beta H_0} e^{-\int_0^\beta \tau V(\tau)}) \]
  \[ Z = \text{Tr}(e^{-\beta H_0} (1 - \int_0^\beta d\tau V(\tau) + \int_0^{\beta_1} d\tau_1 \int_0^{\beta_2} d\tau_2 V(\tau_1) V(\tau_2) + ...)) \]

- Each term is represented by a world line configuration

- **Advantage**: diagonal terms treated exactly
- **Disadvantage**: keeping tracks of times can be computationally expensive

Series Expansion Representation (SSE)

- Based on high temperature expansion, developed by A. Sandvik
  \[ Z = \text{Tr}(e^{-\beta H}) = \sum_{n=0}^{\infty} (-\beta)^n \text{Tr}(H^n) \]
  \[ = \sum_{n=0}^{\infty} \beta^n \sum_{b_1, b_2, ..., b_n} \langle \alpha | \prod_{j=1}^{n} (-H_{b_j}) | \alpha \rangle \]
  with \( H = \sum_i H_i \)

- Similar world line representation but without times assigned

- **Advantage**: easier calculations, no imaginary times needed
- **Disadvantage**: diagonal terms treated perturbatively
More technical details

♦ Example: 1D Heisenberg AFM

\[ H = J \sum_i S_i^x S_{i+1}^x + J \sum_i \frac{1}{2} (S_i^z S_{i+1}^z - S_i^z S_{i+1}^z) \]

♦ Make all matrix elements of \(-H\) positive
  - Add offset to diagonal elements
  \[ -H_{i,i} = -JS_i^z S_{i+1}^z + \frac{J}{4} \]

♦ Gauge transformation on one sublattice for offdiagonal operators

\[ -H_{i,i} = J (S_i^z S_{i+1}^z + S_{i+1}^z S_i^z) \rightarrow (-1)^i S_i^z \rightarrow J (S_i^z S_{i+1}^z + S_{i+1}^z S_i^z) \]

♦ Extend operator string to fixed length \( \Lambda \) by adding extra unit operators:

\[ -H_0 = 1 \quad n \quad \text{... number of non-unit operators} \]

\[ Z = \sum_{n=0}^{\Lambda} \sum_{\{b_i\}} \sum_{\{b_i\}} \sum_{\{a_i\}} \frac{(\Lambda-n)! \beta^n}{\Lambda!} \left\langle \sum_{\{a_i\}} \prod_{i=1}^{\Lambda} (-H_{a_i}) \right\rangle \approx \left\langle \sum_{\{a_i\}} \prod_{i=1}^{\Lambda} (-H_{a_i}) \right\rangle \]

Negative Sign Problem

♦ All the stochastic methods map quantum to classical system

\[ \langle A \rangle = \frac{\text{Tr}[A \exp(-\beta H)]}{\text{Tr}[\exp(-\beta H)]} = \sum_i A_i p_i / \sum_i p_i \]

♦ Sign problem if one of the \( p_i < 0 \) and cannot be gauged away
  - Occurs in fermionic and frustrated problems

\[ \langle A \rangle = \frac{\sum_i A_i p_i / \sum_i p_i}{\sum_i p_i / \sum_i p_i} = \frac{\langle A \cdot \text{sign} \rangle_{\text{ld}}}{\langle \text{sign} \rangle_{\text{ld}}} \]

♦ Exponentially increasing cancellation problem in sign

\[ \langle A \cdot \text{sign} \rangle_{\text{ld}} = \langle \text{sign} \rangle_{\text{ld}} = \exp(-c \beta N) \Rightarrow \Delta A = \exp(+c \beta N) \]

♦ In general harder than NP [MT and U.-J. Wiese]
  - But meron algorithm can solve sign problem in some cases
Step 1: Local diagonal updates

- Diagonal operators can be inserted and removed anywhere
  - In SSE:
    - configuration index
    - operator
    - $P[1 \rightarrow H_{i,d}] = \min \left( \frac{\beta N_{\text{bonds}}(\alpha|H_{i,d}|\alpha)}{L-n} \right)$
    - $P[H_{i,d} \rightarrow 1] = \min \left( \frac{L-n+1}{\beta N_{\text{bonds}}(\alpha|H_{i,d}|\alpha)} \right)$
  - In path integrals:
    - infinitesimal probabilities per time step $d\tau$
    - $P_{\text{insertion}} = H_{i,d} d\tau$
    - like radioactive decay process, we determine a decay time where the diagonal operator is inserted

Step 2a: Offdiagonal updates (local)

- Are very easy, can be done in any representation
  - Problem 1: only local changes
    - Nonergodic
    - No change of magnetization, particle number, winding number
  - Problem 2:
    - Critical slowing down
  - Solution: cluster algorithms
Offdiagonal loop-cluster updates

- Updates form closed loops since world lines may not be broken

![Diagram of offdiagonal loop-cluster updates]

- Introduce graph-representation
  - Connected spins must be flipped together
  - Local configurations:
    ![Local configurations]
    - Local graphs:
      ![Local graphs]

Cluster building rules: Heisenberg antiferromagnet

- Example: XY-like AFM:
  \[
  W(C) = \sum_{G} W(C,G) = \sum_{G} \Delta(C,G) V(G)
  \]

<table>
<thead>
<tr>
<th>\Delta(C,G)</th>
<th>![Configuration 1]</th>
<th>![Configuration 2]</th>
<th>![Configuration 3]</th>
<th>W(C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>[\downarrow \uparrow \uparrow \downarrow \uparrow]</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>[J/2]</td>
</tr>
<tr>
<td>[\uparrow \downarrow \downarrow \uparrow \downarrow]</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>[\uparrow \downarrow \uparrow \downarrow \uparrow]</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>[J_z/2]</td>
</tr>
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- Connected spins form a cluster and have to be flipped together
- Very simple and deterministic for Heisenberg model
Loop algorithm in a magnetic field

- Loop algorithm requires spin inversion symmetry
- Magnetic field implemented by a-posteriori acceptance rate
- Example: spin dimer at $J = h = 1$

Probability $P = \exp(-\beta/2)$

- Triplet
  $E = J/4 - h = -3/4$
- Singlet
  $E = -J/4 = -1/4$

Loop algorithm must go through high energy intermediate state

Exponential slowdown

Worm updates

- Prokof'ev et al 1997 (path integrals), Sandvik 1999 (SSE)
- Insert pair of creation/annihilation operators
  - move these operators (worm head/tail) using local moves
  - when head and tail meet -> have created a loop, update is finished

$H \leftarrow H + \eta(S^+ + S^-)$

- If bounce path can be eliminated $\Rightarrow$ loop algorithm with pre-chosen paths
Worm algorithm in a magnetic field

- Worm algorithm performs a random walk
- Change of configuration done in small steps
- Example: spin dimer at $J = h = 1$

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<th>Singlet</th>
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<td>$E = J/4 - h = -3/4$</td>
<td>$E = -3J/4 = -3/4$</td>
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No high energy intermediate state

Efficient update in presence of a magnetic field

When to use which?

- All algorithms possible in both representations
- SSE usually preferred (computationally simpler)
- Use path integrals only if
  - Large diagonal matrix elements
  - Time-dependent interactions (dissipation or DMFT)
- Use loops if possible
- Use worms if
  - Loops not possible
  - Loops have small acceptance rates

<table>
<thead>
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<th>SSE</th>
<th>Path Integrals</th>
</tr>
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<tbody>
<tr>
<td>Loops</td>
<td>Spin models</td>
<td>Spin models + dissipation</td>
</tr>
<tr>
<td>Worms</td>
<td>Spin models + magnetic field</td>
<td>Bose-Hubbard models</td>
</tr>
</tbody>
</table>
Further problems for Monte Carlo Methods

1. *Critical slowing down* at second order phase transitions
   Solved by Swendsen-Wang cluster algorithm

2. *Tunneling* through *free energy barriers* at first order transitions and for
disordered systems

3. Calculation of the *free energy* $F$ and entropy $S$
   Metropolis algorithm only give transition probabilities
   \[
   W[i \to j] = \min \left[ \frac{p_j}{p_i} \right]
   \]
   Normalization factor (partition function $Z$) unknown
   \[
   p_i = \exp(-E_i / k_B T) / Z \quad F = -k_B T \ln Z
   \]

*Wang-Landau sampling solves all three problems*

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The Wang-Landau method

- Directly calculates density of states $\rho(E)$ instead of canonical average
- Acceptance rate proportional to inverse density of states
  \[
  p_i = \frac{1}{\rho(E_i)} \]
  instead of $p_i = \exp(-E_i / k_B T)$
- Random walk in energy space
  - Flat histogram in energy space => *no tunneling problem*

- *Free energy accessible*
  \[
  F = -k_B T \ln \sum_i \rho(E_i) e^{-E_i / k_B T}
  \]
- One simulation gives results for all $T$

- F. Wang & D.P. Landau
  PRL 86, 2050 (2001),
  PRE 64, 056101 (2001)
Details of the Wang-Landau method

- Initially $\rho(E)$ is unknown
  - Start with $\rho(E)=1$ and adjust iteratively

- Only a few modifications to usual sampling needed
  Start with modification factor $f=1$
  do {
    do {
      Metropolis updates with transition probability $W[i\rightarrow j] = \min[1, \rho(E_i)/\rho(E_j)]$
      Adjust $\rho(E)$ at each step: $\rho(E) \leftarrow \rho(E) \times \exp(f)$
    } until histogram $H(E)$ is “flat”
    decrease $f \leftarrow f / 2$
  } until $f \approx 10^{-8}$

- Comments
  - Initially: multiplicative changes with large $f$ allow rapid crude convergence
  - Finally: small $f$ means no systematic errors, detailed balance

Generalizations and Applications

- $1^{st}$ and $2^{nd}$ order transitions and disorder
  - F. Wang and D.P. Landau, PRL 86, 2050 (2001); PRE 64, 056101 (2001)
- Improved sampling
  - C. Yamaguchi and Naoki Kawashima, PRE 65, 056710 (2002).
- Proteins
- Polymer films
- Continuum simulations
  - M.S. Shell et al., cond-mat/0206461
- Potts model
- Reaction coordinates
  - F. Calvo, Report cond-mat/0205428.
- Quantum problems
  - M. Troyer, S. Wessel and F. Alet, cond-mat/0207138
Quantum version - temperature expansion

- Density of states not accessible directly in quantum case
  - Classical
    \[ Z = \sum_{n=0}^{\infty} e^{-\beta E_n} = \sum_{n} p_n e^{-\beta E_n} \]
  - Quantum
    \[ Z = \text{Tr} e^{-\beta H} \]
- Our method based on high temperature expansion (SSE method by Sandvik)
  \[ Z = \text{Tr}(e^{-\beta H}) = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \text{Tr}(H^n) = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{|\alpha|} \sum_{|\beta|} \sum_{\{a_i\}} \langle a_1 \prod_{r=1}^{n} H_{a_i} | \alpha \rangle \lambda^{(a_i)_{r=1}} \]
  with \( H = \sum_{i} H_i \)
  \[ = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{|\alpha|} \sum_{|\beta|} \sum_{\{a_i\}} \langle a_1 \prod_{r=1}^{n} H_{a_i} | \alpha \rangle \lambda^{(a_i)_{r=1}} \]
  \[ = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} g(n) = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \]
- We sample all orders, basis states and operator sequences
  - Acceptance rates proportional to
    \[ \frac{\langle \alpha | \prod_{r=1}^{n} H_{a_i} | \alpha \rangle}{g(n)} \]
  - Series coefficients to arbitrary order \( \Lambda \)
  - Flat histogram in order \( n \approx E k_B T \)

Quantum version – perturbation expansion

- Instead of temperature a coupling constant can be changed
- Based on finite temperature perturbation expansion
  \[ Z = \text{Tr}(e^{-\beta H}) = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{|\alpha|} \sum_{|\beta|} \sum_{\{a_i\}} \langle a_1 \prod_{r=1}^{n} H_{a_i} | \alpha \rangle \lambda^{(a_i)_{r=1}} \]
  \[ = \sum_{n_{\lambda}=0}^{\infty} \lambda^{n_{\lambda}} g(n_{\lambda}) \]
  with \( H = H_0 + \lambda V = \sum_{i} \lambda \chi^{(i)} H_i \)
  \[ n_{\lambda}(b_1,\ldots,b_n) \text{ counts } \# \text{ of } \lambda \text{ terms} \]
- Update probabilities proportional to
  \[ \frac{(-\beta)^n}{n!} \frac{\langle \alpha | \prod_{r=1}^{n} H_{a_i} | \alpha \rangle}{g(n_{\lambda})} \]
- Series coefficients to arbitrary order \( \Lambda \)
- Flat histogram in order \( n_{\lambda} \) of perturbation expansion
An Introduction to Quantum Monte Carlo Cluster Algorithms

Thermal and quantum phase transition

- Thermal phase transition in 3D quantum Heisenberg antiferromagnet
- Quantum phase transition in bilayer quantum Heisenberg antiferromagnet
- Critical temperature determined to three significant digits in one weekend on a PC

Summary

- Classical cluster algorithms
  - Have enabled high accuracy simulations of classical critical systems

- Quantum cluster algorithms
  - Enable similar accuracy for quantum systems
  - Quantum phase transitions
  - Finite temperature phase transitions

- Sign problem
  - No problem for nonfrustrated bosons and spins
  - Prohibits simulations for fermions and frustrated systems
  - In general harder than NP

- Wang Landau sampling
  - Allows calculation of free energy
  - Tunneling through free energy barriers
  - Effective for 1st order transitions and disordered quantum systems